NsG-416

UNIVERSITY OF PITTSBURGH

SECOND ANNUAL REPORT

FOR

NASA GRANT NsG-416

FOR THE PERIOD

1 MAY 1964 TO 30 APRIL 1965

UNIVERSITY
OF
PITTSBURGH

17 87

VERITAS ET VIRTUS

SUBMITTED BY

THE

SPACE RESEARCH COORDINATION CENTER

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I. The Space Research Coordination Center

The Space Research Coordination Center (SRCC) of the University of Pittsburgh, established in 1963, took as its first goal the buildup of major faculty and facility strength in the Division of the Natural Sciences, to provide a broad and firm foundation for space-related research. This goal, to be attained by Phase I of the SRCC program, has now largely been achieved. The support needed was provided by the National Aeronautics and Space Administration, other Federal Agencies, the Commonwealth of Pennsylvania, and Pittsburgh-based foundations.

In June 1964 the University administration authorized SRCC to plan for a similar buildup of major strength in the School of Engineering, the plan to be put into effect as Phase II of the SRCC program. Action to attain this goal has been initiated under the newly appointed Dean, Harold E. Hoelscher. Our request for a second supplement to Grant NsG-416, combined with funds from other sources, is intended to support Phase II of the SRCC program.

By January 1965 it was clear that, with Phase I coming to a successful close and Phase II off to a good start and likely to follow the same pattern, special attention should be given long-term planning for SRCC. Accordingly, SRCC was restructured for this purpose and Phase III, for meeting the long-range objectives, was put into effect concurrently with Phase II. The activities making up Phase III, which have in fact been going on since SRCC was established but which now receive special emphasis, include the following:

1. Continued strengthening of the science and engineering base, with the aim of rounding out a major national center of science-engineering

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excellence.

2. A sharper focus on space-oriented research, with particular emphasis on rocket, satellite, and space probe experiments.

3. Encouragement of interdisciplinary programs, such as our existing program in bioengineering, in space-related areas.

4. Encouragement of the spin-off of knowledge gained by space-related research and development into early industrial and other use, with increasingly close working relations with the University's Knowledge Availability Systems Center.

It is fortunate that SRCC is actively entering this third phase of its operations just as the NASA-financed SRCC Building is nearing completion (the completion date still stands as 17 May). The new structure will house strongly space-oriented programs of Physics and Chemistry, much of the Department of Earth & Planetary Sciences, the KAS Center, and the SRCC's Director's Office. Moreover, it is physically connected to the University's science-engineering complex.

The Chancellor recently appointed an SRCC Council to work with the Director of SRCC in planning the Phase III activities. The Council's membership is as follows:

SRCC Council

David Halliday (Chairman)	Director (Acting), SRCC; Dean, Division of the Natural Sciences
Wade Fite	Professor of Physics
Arman Frederickson	Chairman, Department of Earth & Planetary Sciences
Harold Hoelscher	Dean, Schools of Engineering and Mines
Putnam Jones	Dean, the Graduate Faculty; Institutional Representative for the NASA predoctoral program

Allen Kent	Director, KAS Center
Niel Wald	Professor of Radiation Health
Campbell C. Yates	Professor of Aeronautical Engineering

The Director of SRCC reports directly to the Chancellor through an advisory committee of Vice Chancellors. These administrative arrangements facilitate involvement of the total institution, faculty and administration alike, in the SRCC program.

II. NASA Predoctoral Trainees

Since the establishment of the Space Research Coordination
Center 43 graduate students have been enrolled or are currently enrolled
as NASA Predoctoral Trainees, under NASA Grant NsG(T)-70. Of these,
two have completed the requirements for the Ph.D.; all others are in
excellent academic standing as Appendix A shows. The two students who
have earned their Ph.D. degree are:

1. John Joseph Farrell (Ph.D) Chemistry

    Thesis: Magnetic Properties of $CeFe_2$, $LuNi_5$, and Some

    1:2 Intermetallic Compounds of Lanthenide Metals

    Position: Assistant Professor of Chemistry at Franklin

    and Marshall College

2. Joseph Bernard Natowitz (Ph.D) Chemistry

    Thesis: Cross Sections and Isomeric Yield Ratios for

    (d,p) and (d,n) Reactions

    Position: Postdoctoral Research Associate at State

    University of New York at Stoneybrook

III.   NASA Postdoctoral Research Associates

Since the establishment of the Space Research Coordination Center fourteen individuals have been appointed as NASA Postdoctoral Research Associates under NASA grant NsG-416. Their names and research program titles are listed in Appendix B.

IV. Capital Construction

1. Van de Graaff building ($1,630,000). This building, designed to house the first three-stage Van de Graaff accelerator, is completed and now occupied. Construction was financed from local private sources.

2. Space Research Coordination Center building ($1,500,000). Construction will be finished by 17 May 1965, and occupancy will be complete by September 1965. The building was financed by NASA Facilities Grant NsG(F)-13.

3. Natural Sciences buildings ($7,405,000). Two buildings are to be constructed with these funds, which have been authorized by the General State Authority. Architects' drawings for the first building, to be built as an extension to the Natural Sciences quadrangle, are complete and occupancy by major portions of the Departments of Biology, Psychology and of Earth & Planetary Sciences is expected by September 1967. The second building, to house the Department of Chemistry, will be erected on an upper campus site on a somewhat later time schedule.

4. Engineering building ($14,600,000). Working drawings for this GSA-financed structure are completed and occupancy is anticipated for late 1967.

V. Research Reports

1. SRCC Reports:

The Space Research Coordination Center has established the policy of circulating reports, in special covers, of space-related research programs at the University of Pittsburgh. Report No. 2, "Rocket Measurements of the Visible Dayglow" by Edward Zipf, Jr., accompanies this report. Report No. 1, currently in preparation, consists of assembled reprints of recent journal articles by our Laboratory Astrophysics group. Reports Nos. 3 and 4, "Low Energy Electron-Atom and Electron-Molecule Scattering Theory Circa 1964" and "Momentum Transfer Theorem for Inelastic Processes," both by Edward Gerjuoy, will be circulated soon.

Much of the research described in SRCC reports was supported in whole or in part by NASA Grant NsG-416. Space-related research supported by other agencies will also be reported, the source of support being made clear in each case. Several newly appointed individuals received necessary initial support under NASA Grant NsG-416 and later developed other support in the form of project grants, either from NASA (as in the case of Professor Zipf) or from other agencies (as in the case of Professor Fite).

Some research reported in the following pages is supported in part by other agencies, this fact being indicated at the appropriate place. In all cases, however,

there is also substantial continuing support from NACA

Grant NsG-416.

2.

POLYSACCHARIDE SYNTHESIS IN CRYPTOCOCCUS LAURENTII
by
Helmut Ankel, NASA Research Associate in Biology

Many microorganisms produce extracellular polysaccharides either in the form of a capsule surrounding the cell or as a slime which is excreted into the growth medium. We have chosen to investigate the biosynthesis of such a polysaccharide in order to obtain information regarding

a) the metabolic pathway which leads to the formation of activated sugar monomers- sugar nucleotides- from which monosaccharide is transferred to polysaccharide,

b) individual enzymes involved in synthesis and interconversion of these sugar nucleotides,

c) metabolic control and regulation of polymer biosynthesis at the enzyme level.

Cryptococcus laurentii, a yeast-like organism produces a capsular heteropolysaccharide composed of mannose, glucuronic acid, and xylose in the molar ratio of 5:1:2. When this project was initiated, the following metabolic pathway leading from glucose to polysaccharide was proposed as a working hypothesis:

Polysaccharide
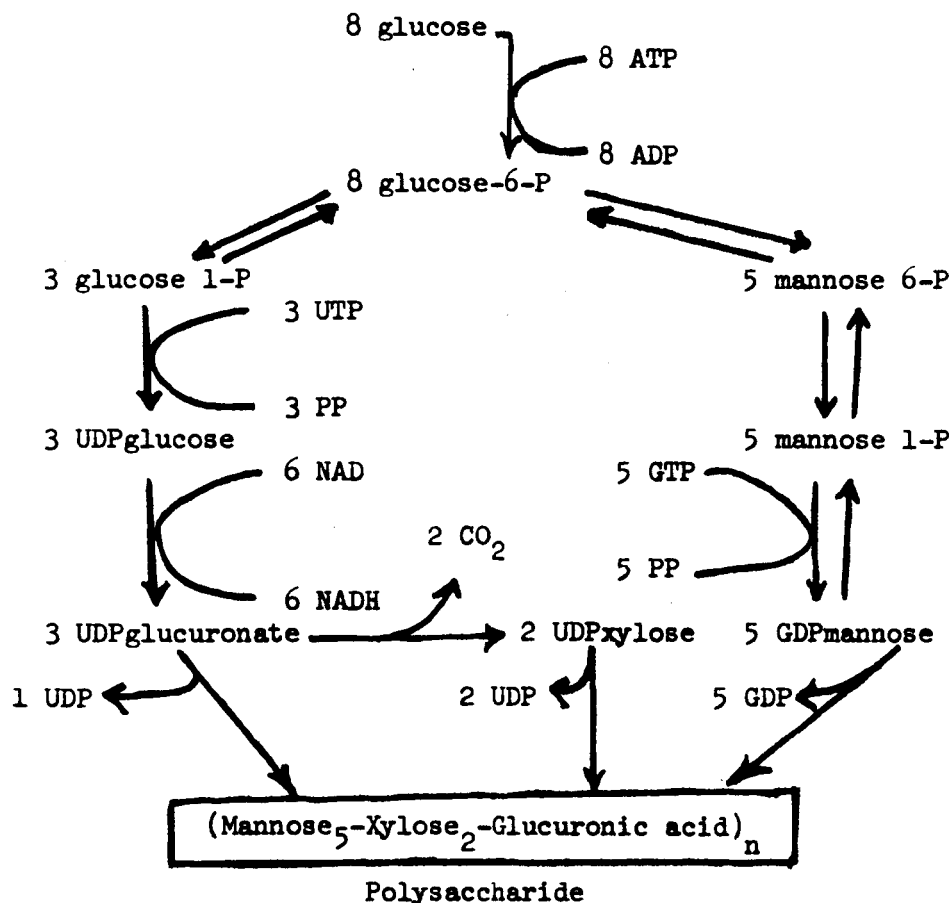
During the tenure of my NASA fellowship I have been able to obtain evidence which substantiates the original hypothesis:

a) The following nucleotides have been isolated from extracts of Cryptococcus laurentii cells: UDP-D-glucose, UDP-D-xylose, and GDP-mannose.

b) The following enzyme reactions have been demonstrated in cellfree extracts:

UDP-glucose + PP $\rightleftharpoons$ glucose 1-P + UTP (UDP-glucose pyrophosphorylase)

GDP-mannose + PP $\rightleftharpoons$ mannose 1-P + GTP (GDP-mannose pyrophosphorylase)

UDP-glucose + 2 NAD $\longrightarrow$ UDP-glucuronate + 2 NADH (UDP-glucose dehydrogenase)

UDP-glucuronate + H^+ $\longrightarrow$ UDP-xylose + CO_2 (UDP-glucuronate decarboxylase)

c) The following enzymes have been partially purified and their enzymatic properties have been studied: UDP-glucose dehydrogenase and UDP-glucuronate decarboxylase.

Results:

a) UDP-glucuronate decarboxylase

Previous results have revealed that the enzyme from Cryptococcus laurentii has an absolute and specific requirement for the addition of catalytic amounts of NAD (K_a = 3 x 10^{-6}M) and that it is competitively inhibited by NADH (K_i = 2 x 10^{-6}M). The same enzyme obtained from wheat germ shows no cofactor requirement and is not inhibited by NADH. The lack of response to the addition of NAD or NADH was thought to indicate that the plant enzyme might contain firmly-bound NAD. Subsequently I have been able to demonstrate that purified wheat germ enzyme contains a nonprotein component, which is released when the enzyme is denatured with heat or acid. This component was shown to be NAD by its enzymatic reduction to NADH, its activating property towards Cryptococcal decarboxylase, and its reactivity with NAD glycohydrolase. The most purified wheat germ decarboxylase contains approximately 1 Mole NAD per 300,000 g protein. In the previous report it was proposed that NAD could act as a reversible H-acceptor in the transient formation of a β-ketoacid. UDP-4-keto-glucuronic acid would easily decarboxylate in analogy to other β-ketoacids. However, when UDP-glucuronate labelled with tritium in the 4 position is used as a substrate, label is retained after formation of UDP-xylose with both enzymes, even in the presence of added NADH. UDP-glucuronate-3-T likewise retains label after decarboxylation with either enzyme, thus excluding enolisation of a transient 4-keto compound with the hydrogen atom at the neighboring C-3. Transient formation of UDP-4-keto glucuronic acid therefore remains hypothetical.

b) UDP-glucose dehydrogenase

        Enzymatic activity of this enzyme is inhibited by low concentrations
of UDP-xylose (K_i appr. 3×10^{-6}M). Although this inhibition can be
overcome by increasing the UDP-glucose concentration, the inhibition does
not appear to be strictly competitive. UDP-xylose shows the typical
characteristics of a feedback inhibitor by which one enzyme of an enzymatic
pathway is inhibited by the product of an enzymatic reaction occurring at
the end of the pathway.

Conclusions:

a) As demonstrated in the scheme (page 9) energy equivalent to 16 moles of
ATP is needed for the formation of one polysaccharide unit. Six moles of
NADH are formed when 3 moles of UDP-glucose are oxidized to UDP-glucuronate.
Since in oxydative phosphorylation 1 Mole of NADH results in the formation
of 3 Moles of ATP, 6 Moles of NADH would correspond to 18 MOLES of ATP, which
would account for all the energy required for the synthesis of Cryptococcal
polysaccharide.

b) Two reactions of the pathway are essentially irreversible, the oxydation
of UDP-glucose and the decarboxylation of UDP-glucuronate. This situation
should eventually lead to an accumulation of UDP-xylose. Yet, in extracts
of the organism UDP-xylose is found only in very small amounts: the ratio
of UDP-glucose to UDP-xylose was estimated to be in the order of 100 to 1.
Since UDP-xylose can act as a strong inhibitor of UDP-glucose dehydrogenase,
in vitro, feedback inhibition by UDP-xylose might be of physiological
significance for the regulation of the UDP-glucose/UDP-xylose ratio.

c) That UDP-glucuronate is not immediately decarboxylated to UDP-xylose,
but is available as a precursor for glucuronate transfer to polysaccharide,
might be regulated in vivo by the NAD/NADH ratio. For every mole of
UDP-glucuronate produced 2 moles of NADH are formed, which would inhibit
further decarboxylation to UDP-xylose. Only when NADH is reoxydized,
presumably via oxydative phosphorylation, can UDP-xylose be produced, and
utilized as a precursor of polysaccharide synthesis.
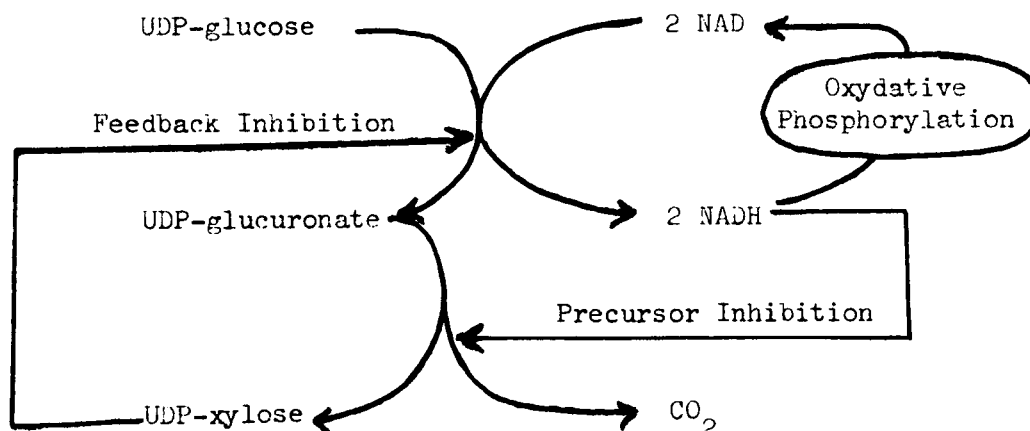
3.

CORRELATION BETWEEN PHYSICAL AND GENETIC DISTANCE
IN INFECTIVE BACTERIOPHAGE DNA
by
D. MacDonald Green, Associate Professor of Biology

In the Second Semi-Annual Report for NASA Grant NsG-416, initial studies were described which correlated genetic map distance with the physical distances of infective DNA molecules. The preliminary studies sought to ask the question whether shearing of whole phage DNA molecules could cause disruption of the linkage of marker pairs carried by the DNA molecule. This was confirmed and, in a general manner, a correlation between genetic map distance between marker pairs and their sensitivity to unlinking by shear was observed.

The present research has extended these preliminary observations. First, it has been possible to produce and characterize DNA molecular fragments that represent quarter, eighth, and possibly sixteenth portions of the original phage DNA molecule, as well as the initially studied half molecules. The use of these smaller fragments for the determination of unlinkage caused by molecular shearing has introduced substantially greater precision into the correlation of map distance and the physical size of the molecule bearing the markers. Secondly, many new marker pairs representing segments of all regions of the genetic map have been examined for their shear sensitivity and a general correlation between map distance and shear sensitivity has been observed for all large (greater than 0.2) segments of the genetic map.

Although a general relationship exists between physical and genetic distances, certain marker pairs that span short genetic distances have been observed to show greater than expected shear sensitivity. Such exceptions can be expected to arise from diverse and interesting sources, such as genetic complexity of markers, a discontinuous distribution of the sites of recombination, high positive interference, or, may reflect an otherwise unexpected "uniqueness" of the phage DNA molecule. These exceptions point out the necessity of scanning short segments of the genetic map for their sensitivity over the entire map.

In conclusion, genetic analysis of phage DNA that has been modally sheared to half, quarter, and eighth molecules shows a good general correlation between map distance and physical size of the DNA. Exceptions to this general observation do, however, occur at small map distances. The reasons for these deviations are being investigated.

4.

GENETIC AND BIOCHEMICAL EFFECTS OF RADIATION ON SOMATIC CELLS
by
S. Venketeswaran, NASA Research Associate in Biology

Somatic cells of different strains of tobacco consisting of
(i) albino mutant maintaining as white non-chlorophyllous tissue;
(ii) unstable albino spontaneously producing chlorophyllous areas; and
(iii) normal green-pigmented tissue are continuously grown as solid and as
liquid suspension cultures. The liquid cultures maintain such an active
growth rate that subculturing is required every three weeks. Since the
submission of the last report in November, emphasis has been directed
towards three major directions:

(1) Comparative studies of gamma radiation effects on callus tissues
growing in liquid suspension vs. fully organized plants (newly-germinated
seedlings):

Detailed data are available of earlier observations on the relative
degree of radiosensitivity of tobacco callus tissue vs. fully organized
plants. The dose of observed morphological effect for callus tissue was
around 7000r (roentgen) whereas only 500r produced an inactive meristem and
stunted leaf growth. The lethal dose for callus tissue was beyond 12,000r
whereas for the meristems it was around 5000r. This difference in
radiosensitivity between the callus tissue and the meristem of fully organized
plants becomes important because these situations may be interpreted to be
analogous to an "open system" vs. a "closed system," i.e., callus tissue
representing the "open system" where the proliferating cells are friable,
noncoherent, loose and free from each other. In comparison, the apical
meristem will represent a "closed system" where the few number of
meristematic cells present at the apex are very compact and under the
influence of the metabolism of the organizational environment of the intact
plant. This high radioresistance of callus tissue in comparison to that of
an organized plant can be a valuable consideration for further studies in
space biology, with respect to expected stability of living organisms in
areas of higher radiation.

The results obtained on this aspect of research are being written
out at present and I am expecting to submit the manuscript to Radiation
Botany, an International Journal devoted to Plant Radiobiology.

(2) Study of chemical and physical factors influencing the development
and continued maintenance of a "chlorophyll system" in cells in culture:

A paper entitled STUDIES ON THE ISOLATION OF GREEN PIGMENTED
CALLUS TISSUE OF TOBACCO AND ITS CONTINUED MAINTENANCE IN SUSPENSION CULTURES
submitted to Physiologia Plantarum (Publn. of Scandinavian Soc. of Plant
Physiology) has been accepted for publication and due to appear around
September 1965.

As indicated in the previous report, the albino callus tissue, although derived from a single-gene mutant and incapable of chlorophyll production under normal conditions, can proliferate "chlorophyllous areas" under specific culture conditions. A series of experiments on tissues derived originally from one single plant (A-1 series) show that indoleacetic acid (IAA) and kinetin, both at 1 x 10^{-6}M favor chlorophyll production and its continued maintenance in culture. The chlorophyll formed is very sensitive to strong light.

A manuscript on the chlorophyll instability of this mutant under varied culture conditions is under preparation.

(3) Cytological and biochemical examination of cells and tissues in culture:

Preliminary cytological analysis of the tobacco tissue cultures reveal abnormal nuclear behavior, cells at different levels of ploidy, etc. Detailed analyses are in progress since nuclear size, structure and composition are important factors in studies on control of radiosensitivity at the cellular and tissue level.

From a biochemist's standpoint, this strain of tobacco tissue shows evidence of extracellular polysaccharide synthesis unlike other tobacco tissues which are in culture in our laboratory. Since polysaccharides are important members of biological macromolecules, detailed biochemical investigations on this strain are needed and efforts towards this are pursued.

Plans for the Immediate Future

(i) Isolation of "single-cell"-clones from chlorophyllous areas of the unstable albino; (ii) extended studies of the effect of white, red and blue light on green-pigmented tissues and (iii) comparative studies of radiation responses of callus tissue vs. meristem to a range of doses of ultraviolet irradiation.

The various aspects of research progress reported here relate to larger programs in the department, especially those directed toward studies of the genetic determination and stability of the photosynthetic mechanism, the effects of radiations on living systems, and the behavior of cells and tissues cultured in vitro.

5.

HYDROPHOBIC BONDING
and
THE STRUCTURE OF THE "HYDRAZONE" OF DINAPHTHOQUINONE
by
Elli Hand, NASA Research Associate in Chemistry, and
Theodore Cohen, Associate Professor of Chemistry

Hydrophobic Bonding

The study of aggregate formation between organic molecules
in aqueous solutions as monitored by n.m.r. and attributed to
hydrophobic bonding has been published as a communication:
"Hydrophobic Bonding. Its Detection by Nuclear Magnetic
Resonance Spectroscopy and Its Effect on the Chemical Shifts
of Internal Standards", J. Am. Chem. Soc., 87, 133 (1965).

The Structure of the "Hydrazone" of Dinaphtoquinone

The structure determination of the alleged hydrazone of
dinaphthoquinone is nearly complete. The highly insoluble
black material has neither Pummerer's structure I nor structure
II which we used as a working hypothesis, but structure III.
While the oxidative degradation products, which have now been
identified, can support either II or III, the acetylated
derivative (IV) of the reduction product obtained by hydrogenation
or treatment with sodium borohydride indicates structure III.
Compound III can be regenerated from IV by basic hydrolysis in
the presence of air.

On the basis of the correct structure it is clear that the
synthesis, outlined in the Second Semi-Annual report, 1 November
1964, and attempted under various conditions without success,
could not have given the "hydrazone". No direct evidence has
as yet been obtained for the anticipated charge-transfer
properties of the compound.
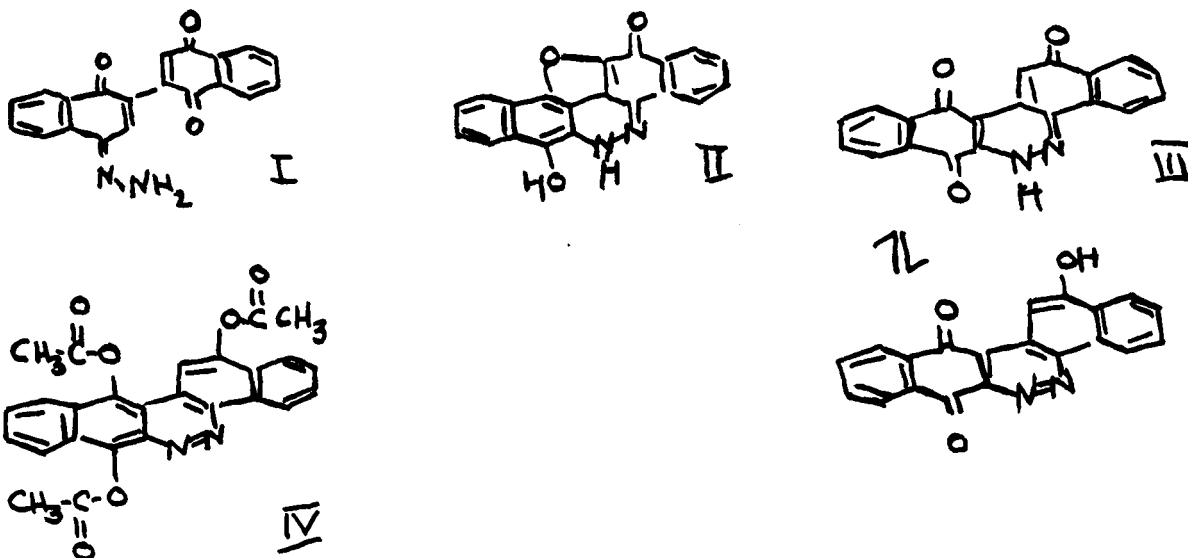
6.

STATISTICAL INFERENCE FROM RADIOACTIVITY MEASUREMENTS
by
Edgar Inselberg, NASA Research Associate in Chemistry

Previous Work

A major part of the 1963-64 year was devoted to work in photosynthesis. Two publications based on this work were discussed in previous reports. During the rest of the 1963-64 year and during the 1964-65 year I have been working on statistical inference from radioactivity measurements. I completed an extensive literature review, familiarized myself with recent developments in instrumentation, including space applications, studied recent textbooks in applied statistics to review the mechanics, underlying assumptions and applicability of various statistical tests, and studied topics in mathematics and mathematical statistics, in preparation for the derivation of a statistical model for the variability of radioactivity measurements.

Statement of the Problem

In measurements of radioactivity, the square root of the total count is often considered to estimate the standard deviation, based on a property of the Poisson distribution, which such measurements are assumed to follow. However, when the activity is estimated by taking the mean of counts of several experimental units, such as planchets, the sample standard deviation is usually significantly greater (as shown by F or chi-square tests) than the value corresponding to the square root of the mean total count. The first type of precision index (square root of the total count) applies to what is commonly referred to as counting statistics, while the second type of precision index applies to what may be called the statistics of radioassay. One of the main objectives of this investigation has been to determine the relationship between counting statistics and statistics of radioassay.

Theoretical Model

The variability associated with a radioassay procedure (statistics of radioassay) can be partitioned into two major components, one attributable to the randomness of radioactive decay (counting statistics) and a second component, which shall be designated as the procedural error.

The variability expected when the same activity is counted repeatedly in a detector free of instrumental fluctuations, and without disturbing sample geometry, corresponds to the component due to the random nature of radioactive decay. The total count, T, is a discrete random variable having the Poisson distribution (neglecting counter dead time effects, which are eliminated by live timing) with a mean value denoted by μ_T and standard deviation, σ_T, equal to $\sqrt{\mu_T}$. Such measurements, however, are of limited value for statistical inference.

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In a typical tracer experiment, several experimental units, such as planchets, are counted, to provide an estimate of the mean of the distribution of the observed total count, R, which shall be denoted by μ_R. In this case several errors are superimposed onto the variability due to the randomness of radioactive decay. These errors are treated as continuous, mostly normally distributed random variables (though further study is needed to establish the nature of the probability distribution of some of the variables). The main procedural random variables are volumetric, or mass errors, variation in the geometric configuration of the sample, and fluctuations within the counter affecting detection efficiency. The procedural random variables all have a mean of zero and standard deviations characteristic of the experimental procedure employed. The procedural error, P, is, therefore, a continuous random variable, apparently normally distributed, with a mean, μ_P, equal to the sum of the means of the procedural random variables, namely zero, and a variance, σ_P^2, equal to the sum of the variances of the procedural random variables.

Thus, the count, R, recorded when several experimental units are assayed is a discrete random variable, equal to T + P (P is manifested as a discrete variable, because the counter records R for any value in the interval R$\leq$ <R + 1). Hence,

$$\mu_R = \mu_T + \mu_P = \mu_T + 0 = \mu_T \qquad (1)$$

while the standard deviation of the observed count, σ_R, is given by

$$\sigma_R = \sqrt{\sigma_T^2 + \sigma_P^2} \qquad (2)$$

The distribution of the observed count, R, is not a Poisson distribution, as shown by its moment generating function, even though it has the same mean as the distribution of T, the Poisson-distributed random variable. The distribution of R is broader and flatter than the corresponding Poisson distribution (has greater standard deviation), and less skewed than the latter. As the procedural error decreases, the generalized distribution of the observed count approaches the Poisson distribution with parameter μ_R as a limiting distribution. The value of σ_R is the starting point for statistical inference.

Validation of the Model

Statistical analysis of data obtained while on a prior position indicates that the model is compatible with experimental findings. A counting system can be evaluated on the basis of σ_P, which is independent of the counting rate, and can be readily determined from the relations given and analogous relations for the counting rate.

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Future Plans

1. To investigate certain aspects of the theoretical model, such as the nature of the probability distribution of some of the procedural random variables which may not be normally distributed.

2. To examine alternative models and determine which model appears to agree best with experimental findings, on the basis of statistical criteria.

3. To examine implications of the model for statistical inference and its applications, for example tolerance limits for radiation, and selection of counters.

4. To determine methods of partitioning the procedural error into its components by the analysis of variance.

7.

THE BEHAVIOR OF HIGH-ENERGY INTERMEDIATES IN ORGANIC SYSTEMS

by

Jack L. Pinkus, NASA Research Associate in Chemistry, and
Theodore Cohen, Associate Professor in Chemistry

Studies concerned with the behavior of carbonium ions of graded reactivity in model systems have been continued. The isolation of a secondary amine in addition to a primary amine, 3 α-amino-5α-cholestane (I), during the ammonolysis of 3 β-tosyloxy-5α-cholestane (II) suggested that a carbonium ion intermediate was involved in the reaction. The stereochemistry of the secondary amine was established as diaxial (di-3 α-cholestanylamine) on the basis of nuclear magnetic resonance evidence. The results of mixed solvent studies in the ammonolysis reaction indicate that the tosylate (II) and the primary amine (I) may be in the form of mixed micelles in the ammonia solution due to hydrophobic-type bonding. An investigation concerned with the generation of carbonium ions by ionization of tosylate II in various media and the reaction of these ions with hindered nucleophile I is planned. These results will allow us to check on our deductions in the mixed solvent ammonolysis reaction.

Attempts to synthesize optically active 1-phenylallylamine (III) as a precursor to a unique carbonium ion have continued. At present we have encountered difficulties in the conversion of 1-phenylallylisocyanate to the amine III, but we are continuing to pursue this line. Following an alternative route[1] to III, we have attempted to convert the corresponding oxime, phenyl vinyl ketoxime, to III with lithium aluminum hydride with poor results. This approach has now been abondened since the reaction was recently investigated in detail[2] and shown not to proceed to the desired amine III as originally claimed.[1]

1. Y. Pocker, Chem. and Ind., 195 (1959).

2. M. Y. Shandala, M. D. Solomon, and E. S. Waight, J. Chem. Soc., 892 (1965).

Publications

T. Cohen, M. Malaiyandi, and J. L. Pinkus, "The Configurational Relationships of the cis-beta-Decalols and cis-beta-Decalylamines," J. Org. Chem., 29, 3393 (1964).

8.

PROGRESS REPORT
by
John Tanaka, NASA Research Associate in Chemistry

A synthetic method was developed for completely deuterated trimethylamine as was reported in the previous progress report. Since that report, the synthesis has been successfully scaled up and enough material was obtained so that some of its physical properties could be determined. An accurate vapor pressure curve and melting point were determined. The molecular weight was determined as confirmatory evidence. The infrared spectrum was determined for the usual region in our laboratories and in the far infrared by Dr. Foil Miller and his group at Mellon Institute. Adducts of the deuterated trimethylamine with borane carbonyl have been made by Dr. James Carter in our laboratories and the infrared spectra determined in an effort to assign the infrared absorption bands. This latter work by Dr. Carter is still in progress.

The failure of some of the methods tried in the attempted synthesis of the deuterated trimethylamine has led to an examination of the Hoffmann elimination mechanism. It has now been shown that the Hoffmann reaction requires much more stringent conditions in solution than it does for dry pyrolysis. It has also been shown in an extension of work previously done by Doering[1] that hydrogen-deuterium exchange does not take place in the unreacted starting material which is held in solution at temperatures much higher than the temperatures usually used for the reaction. This is of interest in the light of our previous work as well as that by Cope[2] which has shown that the exchange takes place to an easily measurable level during the course of "dry" pyrolysis. A postulate has been made to explain this phenomenon and is currently being tested by further experimentation.

The phenylisocyanide work has also been continued. A note was published.[3] Progress since the publication of the note is to be reported at the American Chemical Society meeting in Detroit. The major items to be covered in the paper at the ACS meeting are the reactions which the phenylisocyanide-borane adduct undergoes with ethereal hydrochloric acid and aqueous hydrochloric acid. The reaction of two moles of phenylisocyanide with a half mole of diborane and the reaction of phenylisocyanide with boron trifluoride will also be reported.

1. W. Doering and A. K. Hoffmann, J. Am. Chem. Soc. 77, 521 (1955).

2. A. C. Cope, N. A. LeBel, P. T. Moore, W. R. Moore, J. Am. Chem. Soc. 83, 3861 (1961).

3. J. Tanaka and J. C. Carter, Tetrahedron Letters 5, 329 (1965).

9.

CLATHRATE HYDRATES
by
Truman H. Jordan, NASA Research Associate in Crystallography

The crystal structure analysis of $H_2CO_3 \cdot Et_2O$ had to be abandoned due to an inability to obtain crystals of the compound that are stable for any length of time. The compound is apparently very unstable in the presence of any amount of H_2O.

Data are now being collected on crystals of bromine hydrate.[1] This is a gas clathrate hydrate. It is the only known gas hydrate to crystallize with the tetragonal water lattice. This crystal structure analysis should reveal the nature of the motion or disorder of the bromine molecule inside the water cage.

1. K. W. Allen and G. A. Jeffrey, J. Chem. Phys. 38, 2304 (1963).

10.

CRYSTAL STRUCTURES OF HYDRATES
by
Thomas C. W. Mak, NASA Research Associate in Crystallography

The crystal structure of hexamethylenetetramine hexa-hydrate has been determined using three-dimensional data collected at -20 C. The analysis revealed a novel type of clathrate structure characterised by hydrogen-bonding interaction between the host and guest species. The water molecules form a hydrogen-bonded framework consisting of staggered columns of slightly puckered $(H_2O)_6$ rings cross-linked to one another. Each hexamethylenetetramine molecule is located in a cage within this framework, and is hydrogen-bonded to the water lattice through three of its four nitrogen atoms. A short note on this structure has been submitted for publication in Science.

In our investigation on the hydrates of simple aliphatic amines[1] and related compounds, a preliminary survey of the crystal data has been carried out. Dr. R. K. McMullan and I have collected a complete set of intensity data on tetramethylammonium hydroxide pentahydrate, and efforts are being made to solve its crystal structure.

A paper on the structure of the tetrahydrofuran/hydrogen sulfide double hydrate[1] has been written and accepted for publication in the Journal of Chemical Physics.

1. Thomas C. W. Mak, Second Semi-Annual Report, November 1, 1964.

11.

INVESTIGATION OF THE SCATTERING OF SEISMIC WAVES FROM GEOLOGIC DISCONTINUITIES

by

Walter Pilant, Associate Professor of Geophysics
Department of Earth & Planetary Sciences

Work on the reflection and transmission coefficients of Rayleigh waves around an edge is still underway. There was a delay while an additional piece of equipment was purchased to give a stable electronic delay to cancel the acoustical delay inherent in seismic modeling techniques. First results show qualitative agreement with the theoretical first order approximation which shows antisymmetry about 180°, i.e., no edge. Also a computer program was written to linearize data obtained from non-linear time sampling and to determine the linearity of the oscilloscope digitization equipment.

During work with the seismic models, which are thin-plate approximations to two-dimensional wave propagation, a dispersion of the surface waves was observed which is apparently due to the finite thickness of the plate. Further investigation of this phenomenon will be carried out in the near future.

In addition to the model seismology experiments, additional financial support has been obtained from an Air Force grant to proceed on the larger problem which includes the analysis of real seismic surface waves. This support will allow the reduction and analysis of data collected by the world-wide network of standardized seismic stations operated by the U. S. Coast and Geodetic Survey. Data from this source will be used to compare with that obtained from the model seismic studies which have been underway in order to provide a more accurate model of the structure of the earth's crust and upper mantle.

12.

PROGRESS REPORT
by
R. Stoneley, Professor of Geophysics
Department of Earth and Planetary Sciences

Since the last report my research work has been concerned mainly with (i) surface elastic waves in anisotropic media, (ii) earth tides.

(i) A paper on the propagation of surface and body waves in a medium with orthorhombic symmetry has been published: the geophysical interest is that if the Earth's mantle, thought to consist largely of olivine, possesses marked anisotropy, then this should show up in variations of wave-velocity with direction. The absence of such variation shows that any such anisotropy is masked by the random orientation of crystal aggregates.

A paper on the polarisation of S-waves in an isotropic medium, regarded as the limit of a cubic medium, has now been published. This verifies a conjecture that two of the three types of waves in a cubic medium degenerate to two distortional waves polarised in different planes.

An investigation of surface waves along the interface between two cubic media is being carried out, with marked success, by Mr. W. Johnson under my direction.

(ii) The wide discrepancies in earth tilt measurements in different regions may possibly depend on regional variations in the crust. To estimate the order of magnitude involved a simplified example has been investigated mathematically, in which there is a periodic variation of rigidity in the mantle.

The Committee of the International Seismological Summary has been much occupied with the setting-up of the International Seismological Research Center; this involved a meeting of the I.S.S. Committee last November in Edinburgh. My report, as Chairman, will shortly be published in the U.G.G.I. Chronicle, the organ of the International Geodetic and Geophysical Union.

An article on "Tsunamis" is awaiting publication by the Pergamon Press.

13.

EARTH TIDE STUDIES
by
R. D. Wyckoff, Professor of Geophysics
Department of Earth and Planetary Sciences

Instruments

The LaCoste-Romberg earth tide gravimeter has been on order for about twelve months. As of February the manufacturers reported the assembly practically complete and that testing could be started in a short time. Since the resolution of the instrument will be better than $10^{-9}g$ the test period could be quite prolonged since minute details of construction and assembly are involved and the long-term drift characteristics of the springs must be determined. Delivery could be expected in May.

In order to have available a complete complement of equipment for tidal measurements a pair of high-sensitivity tilt meters was purchased from the Royal Observatory of Belgium and received in September, 1964. These Verbaandert/Melchoir Type II horizontal pendulums are of all-quartz design and are probably the best instruments of the type presently available. The equipment is complete with photo-recorder and calibration devices. Ultimately, as is true of the gravimeter, they should be adapted for digital recording.

Unfortunately one of the 40 mm. quartz suspensions of one instrument was broken in transit. It did not appear judicious to return the instrument for repair but suitable quartz fibres are available. Repair will be done when suitable facilities and observation site are available.

Earth-tide Observation Site

The tidal gravimeter will require no very special site selection as regards ground stability. On the other hand the tilt meters with a resolution better than 0.001 seconds of arc require an extremely stable, generally solid rock environment. Such a site is not presently available locally. However, significant tidal data is obtainable from the gravimeter alone as is frequently necessary because of environmental conditions.

Geophysical Laboratory Site

Since about November 1964 the University has had available an abandoned Nike Control location about 15 miles from the campus comprising eight acres adequately fenced. In order to test the suitability of the site as a laboratory for seismological and related geophysical studies, one of the small buildings was repaired, equipped with suitable controlled electric heating and seismic equipment temporarily installed. The instruments comprise a Benioff Vertical, two Wenner horizontal pendulums, associated galvanometers together with a 3-drum 24-hour photo-recorder. These are old instruments which when reconditioned appeared suitable for ambient noise level test purposes.

This equipment has been operated more or less continuously for the past several months using the concrete-slab floor of the small one-story concrete block building for the instrument support. Accordingly, the tests are handicapped by inordinate building and wind noise as compared to a proper underground vault with isolated piers. However, recent approximate calibrations of the Vertical Seismometer indicate that in the absence of heavy wind the ambient ground "noise" amplitude is on the order of 1×10^{-5} mm in the 1-2 cps. range suitable for first arrival p-wave detection. Satisfactory operation of the Benioff vertical at a magnification of around 17,000-20,000 in this frequency range indicates that the Nike Site should be quite suitable for normal teleseismic laboratory purposes, especially if provided with the usual underground instrument vault.

As yet I have found no satisfactory facilities to calibrate the horizontal pendulums although distant earthquakes have been satisfactorily recorded. The instruments are operating at 10-second periods with 15-second galvanometers and attenuated to limit the microseismic noise to tolerable levels. The predominant microseisms are in the usual range of 5-6 second periods and any final ambient noise tests would require a sharp elimination filter at this frequency. Moreover, wind noise in the present building environment is a major additional disturbance which would be largely eliminated by a vault. However, these instruments along with the vertical seismometer, indicate that with a vault built into the hill about 20 feet below the upper ground level, the Nike Site would be quite suitable for teleseismic laboratory purposes, as well as other geophysical observations.

Shop Facilities

When space in the new building is acquired we will have available the nucleus of shop-facilities suitable for normal repair and experimental development work. The lathe, vertical milling machine, drill press and associated small bench tools are intended to serve only as laboratory tools without which research is severely handicapped. Job shops for major work are available elsewhere.

Miscellaneous

When called upon I have provided some assistance with instrumentation problems involved in miscellaneous projects. Presently this includes preliminary consideration of certain equipment for oceanographic use.

14.

GENERAL RELATIVITY

by

Alan H. Thompson, Assistant Professor of Mathematics

I. INTRODUCTION

The group whose work is here reported consists of myself and two research students, Mr. R. Reynolds and Mr. R. Roman.

Since the last report two papers have been submitted for publication:

a) A Class of Related Space-Times.

b) On Projective-Symmetric Spaces. (with R. Reynolds)

Also a joint paper with Dr. G. Williams (University of Florida) Space-Times with Corresponding Geodesics, was read at the Annual Meeting of the American Mathematical Society, Denver, January 1965. An abstract appears in Dr. Williams' contribution to the last N.A.S.A. report.

Mr. Roman and Mr. Reynolds are currently occupied in preparation for the Ph.D. preliminary examinations of this Institution. Present work and future programmes will now be outlined.

2. A Class of Related Space-Times.

R. P. Kerr and A. Schild $\begin{bmatrix} 1 \end{bmatrix}$ have considered a space-time $\begin{bmatrix} 2 \end{bmatrix}$ for which the metric tensor can be written

$$(2.1) \qquad g_{ab} = \eta_{ab} + k_a k_b,$$

where η_{ab} is the metric of Minkowski Space in coordinates which are

Cartesian but not necessarily rectangular. The vector field k^a (k_a) is everywhere tangent to a congruence of null curves in the space-time. From (2.1) it follows that $g_{ab}k^b = \eta_{ab}k^b$, and consequently $k^a(k_a)$ is also a null vector field of the associated Minkowski space. For the contravariant form of the metric relationship (2.1) we have:

$$(2.1a) \qquad g^{ab} = \eta^{ab} - k^a k^b.$$

We consider the general relationship of two space-times V_4 and $\widetilde{V}_4$ whose metric tensors, g_{ab} and $\widetilde{g}_{ab}$ respectively, are connected by

$$(2.2) \qquad g_{ab} = \widetilde{g}_{ab} + k_a k_b.$$

where k_a is regarded initially as defining a null covariant vector field in $\widetilde{V}_4$. With (2.2) a short calculation gives

$$(2.2a) \qquad g^{ab} = \widetilde{g}^{ab} - k^a k^b,$$

where $k^a = g^{ab}k_b = \widetilde{g}^{ab}k_b$, and consequently the vector field $k_a(k^a)$ is also a null field of the space-time V_4. The equations (2.2) and (2.2a) imply the relation

$$\Gamma^a_{bc} = \widetilde{\Gamma}^a_{bc} + \widetilde{g}^{ad}\left\{ k_b k_{[d\,\|\,c]} + k_c k_{[d\,\|\,b]} \right\} + k^a\left\{ k_{(b\,\|\,c)} + k_{(b}\,q_{c)} \right\} ,$$

for the connexions Γ^a_{bc} and $\widetilde{\Gamma}^a_{bc}$ of the space-times V_4 and $\widetilde{V}_4$ respectively. Here " $\|$ " denotes covariant differentiation in V_4, and q_c ($= k_{c\,\|\,b}k^b$) is the first curvature vector of the congruence k_c regarded as a vector field of V_4.

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Kerr and Schild have constructed all vacuum solutions ($R_{ab} = 0$) for a space with metric of the form (2.1). A fundamental result for such spaces is that they are _algebraically special_ in the sense of the Pirani-Petrov classification [3]. We will consider the generalisation of this result for the space-times V_4 and $\widetilde{V}_4$ which are subject to the relation (2.2). The following is a summary (without proof) of the main results obtained.

I. The first curvature vector of the congruence k_c is invariant under the transformation $\widetilde{V}_4 \Longrightarrow V_4$: i.e. $q_c = k_{c\|b}k^b = k_{c;b}k^b$ where " ; " denotes covariant differentiation in the V_4. An immediate consequence of this result is that if k_a is a geodesic congruence of $\widetilde{V}_4$ then it is also a geodesic congruence of V_4.

II. The expansion of the congruence k_a is invariant under the transformation $k_a \in \widetilde{V}_4 \Longrightarrow k_a \in V_4$. The optical scalars; shear σ and rotation ω associated with the congruence in the two space transform as

$$\sigma^2 = \widetilde{\sigma}^2 - 1/2\, q^a q_a , \qquad \omega^2 = \widetilde{\omega}^2 + 1/2\, q^a q_a .$$

Consequently for a geodesic congruence k_a these scalars are also invariant. (For a discussion of the terms "expansion" "shear" and "rotation" as applied to a null congruence see the work of W. Kundt [4] and R. K. Sachs [5].)

III. If the spaces $\widetilde{V}_4$ and V_4 are assumed to be special Einstein space ($\widetilde{R}_{ab} = R_{ab} = 0$.) then the congruence k_a is necessarily geodesic.

IV.   For $\widetilde{V_4}$ and V_4 special Einstein spaces, then V_4 is algebraically special with k_a as a double Debever vector if and only if $\widetilde{V_4}$ is algebraically special with k_a as a double Debever vector. (This generalises the result obtained by Kerr and Schild [1])

By weakening the restrictions on $\widetilde{V_4}$ and V_4 we hope to obtain more general statements of the above results.

3. Construction of Exact Solutions of the Einstein Field Equations.

The form of the metric tensor of a special Einstein space (2.1) considered by Kerr and Schild [1] can be systematically generalised in the following manner. We consider the eigen-value equation for a symmetric tensor s_{ab} relative to the Minkowski metric tensor η_{ab}

$$\| s_{ab} - \lambda \eta_{ab} \| = 0.$$

For η_{ab} of signature $+2$ the degenerate cases are given by the Segré characteristics $[211]$, $[31]$ and their subclasses $[(211)]$ and $[(31)]$. For s_{ab} of Segre characteristic $[(211)]$ we have the canonical form

(3.1) $s_{ab} = \lambda \eta_{ab} + k_a k_b$, with k_a null.

The special case $\lambda = 1$, is that considered by Kerr and Schild. For the characteristic $[(31)]$ we have the canonical form

(3.2) $s_{ab} = \lambda \eta_{ab} + 2z_{(a}k_{b)}$,

where k_a is null, and z_a is space-like with respect to the metric η_{ab}. Also they are orthogonal to each other. The relations (3.1) and (3.2) suggest the following generalisations of the work of Kerr and Schild.

We consider a space-time V_4, the metric tensor of which is given by

$$(3.3) \qquad\qquad g_{ab} = e^{2\sigma} \eta_{ab} + k_a k_b,$$

or

$$(3.4) \qquad\qquad g_{ab} = e^{2\sigma} \eta_{ab} + 2z_{(a} k_{b)},$$

where the vectors k_a, and z_a satisfy the same orthogonality relations as in (3.1) and (3.2) and σ is an arbitrary function of the coordinates. It is proposed to calculate the classes of special Einstein spaces (gravitational field in vacuo) whose metric tensor can be expressed in the above forms.

4. Projective-Symmetric Spaces.

The authors Gy. Soos [6] and B. Gupta [7] have considered the class of Riemannian spaces V_n (n > 2) for which the first covariant derivative of the projective-curvature tensor of the space vanishes. Such spaces they call Projective-Symmetric, and their work is concerned mainly with the generalization of results which are true for a symmetric space [8]. We have shown that for the Riemannian case all projective-symmetric spaces are symmetric, and consequently the results of the above authors follow immediately. The more important results that we have obtained are as follows:--

I. In the Riemannian case, all projective-symmetric spaces are symmetric in the sense of Cartan [8].

II. For an affine space with symmetric connexion, A_n (n > 2) there exist projective-symmetric spaces which are not symmetric.

III. A projective-symmetric A_n which is decomposable [9] in necessarily a symmetric space.

IV. For a Weyl Geometry W_n [10], a projective-symmetric space is necessarily a symmetric space.

5. The Shear-free Motion of a Fluid in Space-Time.

An introduction to this problem was presented in the Supplemental NASA report, 1964. It was there suggested that an approach to the problem could be made by means of a conformal transformation from a space containing a rigid congruence of time-like curves. (See for example the work of Pirani and Williams [11].) Unfortunately, though one can in general associate a shear-free motion with a rigid motion (in this manner), the integrability conditions cannot be obtained. (This is apparently due to the fact that a four-index tensor with the symmetries of the Weyl Conformal Curvature Tensor [12] is, in a three-dimensional space, necessarily zero.)

However given a general non-null vector field in space-time u^a, we can associate with this the set of vectors e_μ^a ($\mu = 1,2,3.$) such that $u_a e_\mu^a = 0$, all μ. If the congruence u^a is irrotational, then the set e_μ^a spans a three-dimensional hypersurface embedded in the space-time; if the rotation of the congruence is <u>not</u> zero then the field u^a will not define a system of hypersurfaces of the space. However one can interpret the domain of the vector fields e_μ^a ($\mu = 1,2,3.$) as an <u>Anholonomic</u> $V_4{}^3$ within the space-time. (For general reference to such concepts see the work of Schouten [13].) We hope to use the concept of an <u>Anholonomic</u> $V_4{}^3$ to obtain the results of Pirani and Williams [11] by covariant methods, and then to seek application to the general problem of a space-time admitting a shear-free motion.

6. Spaces with Double-Recurrent Curvature Tensor

An attempt to construct space-times for which the curvature tensor R_{abcd} satisfies a condition of the form

$$R_{abcd;ef} = k_{ef} R_{abcd},$$

was initiated in the last report. The discussion was limited to the vacuum case ($R_{ab} = 0.$) and the object was to obtain new solutions of the gravitational field in vacuo. Some interesting geometrical results were obtained but it was discovered that the class considered was identical with the "class of plane-wave solutions with parallel rays" previously discussed by W. Kundt [14]. The results further suggested that a discussion of the space-times for which

$$P_{abcd;ef} = K_{ef} P_{abcd}; \quad R_{ab} = 0,$$

might lead to hitherto unknown solutions of the Einstein vacuum field equations. Here P_{abcd} is the "complexified" Riemannian Curvature Tensor of Kundt [14], and K_{ef} is not necessarily real.

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THEORETICAL STUDY OF FLOW SEPARATION
by
R. K. Duggins, NASA Research Associate in Mechanical Engineering

A theoretical analysis of flow separation has continued, and considerable progress has been made towards achieving the ultimate objective, viz., the fusion into a single composite unit of the two distinct potential flow theories hitherto used to describe regions of separated flow.

The two theories are the classical free streamline theory and the trapped vortex theory. Application of the former gives a fairly accurate definition of the profile of the dividing streamline, whereas the latter gives a better description of vorticity distribution and a better representation of the reattachment process which often forms a sequel to flow separation. It has been confirmed in the current investigation that many of the attractive features of the two basic theories will be retained in the composite one when the latter is applied to a wide range of flow separation problems.

In the method of analysis being developed, the separation region is considered to be an integral part of the total flow pattern, a vortex sheet being assumed to separate the initial part of the separation region from the main flow stream. The remainder of the vorticity is taken to be trapped in the separated fluid and concentrated at the point centre of the circulatory flow within the region. The location of this vortex centre and the complete distribution of vorticity are uniquely determined in the course of satisfying various stability requirements. A feature of the new method is that only one item of empirical data is required for completion of the solution; the size of the separation region is governed by the point at which the main flow stream reattaches to the bounding wall, and this point is located by experimental pressure measurements.

It seems likely that the type of flow problem to which the newly developed theory will be most appropriate is that in which the flow stream contracts prior to separation, and in which separation occurs at a clearly defined point. Typical geometrical configurations which exhibit these flow characteristics are the sudden contraction and the elbow bend, so these have been chosen for the initial application of the composite theory.

16.

REPORT OF ATOMIC BEAM LABORATORY ACTIVITIES
by
W. L. Fite, Professor of Physics,
R. T. Brackmann, Research Assistant
Professor of Physics and Electrical Engineering, and
W. R. Henderson, Research Associate in Physics

During the past six months the atomic beam laboratory
has made very satisfactory progress both in prosecuting existing
programs and in obtaining support for programs which we had
wanted to undertake. We summarize each of these in turn.

A. Heavy Ion Collisions. The experimental program on the study
of charge changing collisions of heavy ions in gases proceeded
well during the fall and early winter and the entire series of
measurements of Fe^+ in N_2, O_2 and Ar were completed. The energy
range of 50 to 500 kev was again used.

The principal points of interest have come through the
comparison of Fe^+ and Al^+ as the primary ions in collisions with
the various gases. While again it was observed that stripping
of a metallic ion to form a doubly (or higher) charged ion is
much more prominent than for the more usual cases where the
primary ion has a higher second ionization potential, it has
been particularly surprising to find that when the target gas
is molecular the stripping cross section exceeds the charge
capture cross section but when the target gas is Ar, the
stripping cross section is substantially less than the capture
cross section. This strong apparent dependence of the stripping
cross section on whether the target gas is atomic or molecular
is not understood, but if a general pattern of this nature is
found with other metallic ions several interesting consequences
for upper atmosphere phenomena will follow.

These experiments were suspended following the Fe^+
measurements to accommodate other needs for both the 500 kev
Van de Graaff machine and the vacuum system being used. In
recent months the only activity in this program has been the
development of a U^+ ion source for the next series of measure-
ment. This new series should commence in about another month,
and run through most of the summer.

This work is supported by General Dynamics/General
Atomic as a portion of their prime contract with the Air Force
Special Weapons Center.

B. Hydrogen Atom Collisions. This program was funded effective
October 1 by the National Science Foundation. Since its level of
support was substantially below that requested it has necessarily
proceeded somewhat slowly. The major activity has been the

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purchase of those components which are commerically available and
the design and fabrication of the many more components which are
not purchasable.

At this point, the vacuum pumps, traps, etc., are in hand
and early in April the main vacuum chamber system (three-stages)
was delivered. At present the vacuum system is being assembled
and the remaining parts of the control circuitry etc. are being
fabricated.

It has not yet been finally determined which of several
very important experiments will be carried out on this apparatus
first upon its completion. Present inclinations are to under-
take excitation of Lyman alpha radiation using a narrow energy
spread electron gun (which, incidentally, is in existence) as
the first problem.

This program is funded under NSF Grant No. GP 3593.

C.   Electron Collisions with Excited Molecules. The program for
study of collision properties of excited states of molecules was
prompted by the observation that the cross section curve for
dissociative attachment shifts by a dramatic 2 ev only upon
heating the O_2 to a gentle 2000°K (1/6 ev). Such a dramatic shift
suggested that collision cross sections for excited molecules
could vary from those for groundstate molecules by perhaps orders
of magnitude. A proposal to examine this thesis was approved by
the Defense Atomic Support Agency and the Army Research Office
(Durham) and this program was funded on December 1, 1964.

Extremely gratifying progress has been made on this
program in the four months of its existence. The details of
dissociative attachment from excited O_2 are rapidly becoming
known from the modulated crossed beam experiments being performed
with the small atomic beam machine constructed with SRCC funds.
It does indeed seem that dissociative attachment cross sections
have magnitudes which depend strongly on the state of excitation
(i.e., an increase by a factor of several hundred for excitation
levels of about 1 ev). Further, for dissociative attachment at
a given electron energy all states above some minimum state have
the same values for the cross section. These findings appear to
establish an unexpected pattern which will be of aid in the further
development of collision theory and which have direct application
to a number of high temperature phenomena. In addition, it seems
clear that the effect does not require electronically excited
states, but that probably rotational and vibrational excitation
is responsible for the effects.

To date these experiments have not used the monoenergetic
electron gun which was constructed by Dr. Henderson using SRCC
funds. We anticipate that shortly the present electron gun will

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be replaced by the monoenergetic gun and that considerable detail
on the dissociative attachment process will be obtained fairly
rapidly.

This work is supported by Grant No. DA-ARO-D-31-124-G627
from the Army Research Office (Durham).

D. Neutral-Neutral Reactive Collisions. A program to study,
using modulated crossed beam techniques, collisions between
molecules and free radicals in which chemical reactions occur,
was proposed last spring as a major part of the overall activities
of the Atomic Beam Lab. Of primary interest in this proposed
program was the study of certain of the neutral-neutral reactive
processes believed to be responsible for the excitation of the
earth's night airglow and certain auroral phenomena. We are
pleased to report that this program will commence on May 1, it
being funded through the Space Sciences Division of NASA. Since
much of the basic apparatus is similar to that being assembled
in connection with our atomic hydrogen collision program, we
anticipate that accumulation of the necessary equipment for this
program will proceed quite rapidly.

Miscellaneous. During the period October 25 - November 5, W. L.
Fite visited the Soviet Union as an invited guest of the Academy
of Sciences of the U.S.S.R., for the purpose of visiting
laboratories working in the area of atomic collision phenomena
and lecturing. Places visited included the A. F. Ioffe Physical
Technical Institute, Leningrad; Leningrad State University;
Physical Technical Institute of the Ukranian S.S.R., Kharkov;
and Institute for Chemical Physics, Moscow.

Personnel: Personnel involved in the programs of the
Atomic Beam Laboratory are Drs. W. L. Fite, R. T. Brackmann,
W. R. Henderson and Mr. William R. Ott.

17.

ATOMIC PHYSICS--THEORETICAL
by
Edward Gerjuoy, Professor of Physics

The paper, "Multiple-Wave Propagation and Causality," referred to in the last Semi-Annual Report, has appeared in the Annals of Physics, 32, 1-45 (1965). Reprints of this paper will be issued as a report of the Space Research Coordination Center. Other completed papers during the past six months include the review, "Electron-Atom and Electron-Molecule Scattering Theory Circa 1964," also mentioned in the last Semi-Annual Report, which was presented at the January, 1965, New York meeting of the American Physical Society; and "Momentum Transfer Theorem for Inelastic Processes." Abstracts of this last paper, and of the Annals of Physics paper, follow. The review, being a review, requires no abstract; its title thoroughly describes its contents.

* * * *

Multiple-Wave Propagation and Causality

The implications of the principle of causality (loosely stated, that the response to an incident signal cannot begin until the signal arrives) are investigated for the transmission and reflection of electromagnetic waves by multiple-wave media (i.e., media, such as plasmas, which can propagate waves of several different wave numbers $\underline{K}$ (ω) at the same frequency (ω). Although many of the results obviously have wider validity, for concreteness the paper takes the medium to be in fact a plasma, while for simplicity the analysis is restricted to the special case of one-dimensional wave propagation along $\underline{z}$, with the plasma confined to a finite slab $0 \leq z \leq d$. The plasma may be lossy, need not be uniform, and may be stable or unstable. The conclusions drawn include: Causality can be preserved even though the transmission amplitude $\underline{T}$ (ω) and reflection amplitude $\underline{A}$ (ω) have singularities in the upper half ω-plane. Poles of $\underline{A}$ (ω), $\underline{T}$ (ω) in Im $\omega > 0$ typically occur with slabs of unstable plasma. In stable plasmas, the existence of a branch point at Im $\omega > 0$ for one $\underline{K}^2$ (ω) implies there is at least one other $\underline{K}^2$ (ω) with the same branch point. In stable plasmas it is impossible to excite one such nonsingly-valued K^2 (ω) wave without exciting at least one other such wave. With isotropic plasmas the singularities of $\underline{T}$ (ω), $\underline{A}$ (ω) in Im $\omega > 0$ are symmetrically located about the imaginary axis. Despite some complications associated with the limiting behavior of the dispersion equation at infinite $|\omega|$, under ordinary circumstances, with slabs of stable plasma, $\underline{A}$ (ω) and $\underline{T}$ (ω) - 1 each should obey Kramers-Kronig relations. The results are illustrated by reference to two actual plasma dispersion relations--the warm collisionless plasma (stable) and the two-stream plasma (unstable).

Momentum Transfer Theorem for Inelastic Processes

ABSTRACT

        Recently it has been shown that for potential scattering, the
well known optical theorem--relating the total cross section to the
imaginary part of the forward scattering amplitude--can be generalized
to yield a "momentum transfer cross section theorem." The present
paper further generalizes the previous potential scattering result.
Specifically, it appears that the momentum transfer cross section theorem
is valid also for many-particle systems, wherein inelastic processes
occur. Although this last assertion probably holds quite generally, a
proof is given only for the collisions of electrons with atomic hydrogen.
The proof takes into account electron indistinguishability, as well as
the possibility that the incident electron ionizes the atom, but assumes
the forces are not spin-dependent.

                        *   *   *

        During the next six months I shall be working on various
theoretical problems bearing on methods for calculating atomic cross
sections. In particular, there is in preparation a review on methods
of constructing variational principles for arbitrary matrix elements of
arbitrary operators. Some of this and other future work will be
supported by ONR and AFOSR contracts.

17a.

MEASUREMENTS OF CHARGE EXCHANGE AND IONIZATION CROSS SECTIONS
by
Kotu Lulla, NASA Research Associate in Physics

The total charge exchange, $\sigma_{01} + \sigma_{0-1}$, cross sections for neutral atomic hydrogen beam traversing CO have been measured to check the overall performance of apparatus. The results are in fair agreement with previous measurements.[1] The measurements of cross sections for the production of O^- and other products of collision left behind are underway. These results will throw light on processes responsible for structure in the energy dependence of the cross section σ_{0-1}.

The slow ions formed undergo elastic collisions with the gas in the detection region. The ion flux $I(O^-)$ should satisfy,

$$I(O^-) = K_1 I(H)\, n(CO)\, \sigma_{0-}\, \exp - K_2 N\sigma$$

in the low density approximation, assuming ion production is a direct process. In this equation K_1, K_2 are constants depending upon the geometry of the apparatus; K_1 also depends upon the efficiency of ion multiplier. The other quantities are:

N = total gas density in the detector chamber,

σ = the elastic collision cross section,

σ_{0-} = O^- production cross section.

The value of K_1 is extremely complicated to calculate and hence the relative values of cross sections will be compared to some known value of ion production cross section.

In the near future we plan to conduct similar studies for gases such as O_2, H_2, etc.

The construction of the crossed-beam apparatus for the study of charge exchange in $H(30\ kev) + H^+(50-400\ kev)$ collisions is in its final stage. All the electronics for the detection system have been completed.

1. D. V. Philipenko and Ya. M. Fogel, J. Exptl. Theoret. Phys. (U.S.S.R.) 42, 936-943 (1962).

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18.

OPTICAL STUDIES OF ELECTRON AND HOLE TRAPPING LEVELS IN QUARTZ*
by
Mordechay Schlesinger, NASA Research Associate in Physics

ABSTRACT

Illumination with monochromatic light into various color-center absorption bands of quartz at liquid nitrogen temperature (LNT) after previous X-ray irradiation at room temperature (RT) re-excites some glow peaks of the "usual" glow-curve in the region between LNT and RT. Re-excitation can also be performed for peaks above the temperature at which the crystal was x-irradiated. The effect has been investigated in detail for crystals doped with various impurities and under various conditions. The results are in agreement with the generally accepted models for the electronic processes in Quartz.

19.

SOME OPTICAL AND ELECTRICAL PROPERTIES
OF SYNTHETIC "AMETHYST" QUARTZ."
by

Moderchay Schlesinger, NASA Research Associate in Physics,
Alvin J. Cohen, Professor of Geochemistry,
Department of Earth and Planetary Sciences, and
H. L. Pollak, Research Assistant,
Department of Earth and Planetary Sciences

Some of the optical effects of synthetic amethyst grown
by Sawyer Research Products, Inc. along with their electrical
properties were investigated. Color center absorption bands are
present at the wavelengths 1600, 950, 545, 415, and 347 mμ. The
last one is complex, and consists of at least two components,
one peaking at 357 and the other at 343 mμ, polarized in the
parallel (π) and in the vertical (δ) directions to the c-axis,
respectively. The various color centers bleach out thermally at
about 430°C. accompanied with a blue thermoluminescence.
Direct-current polarization effects have been observed in the
amethyst crystals. The sample was subjected to a dc "step"
potential and the transient polarization currents recorded. The
effect was studied both in the "colored" and in the "bleached"
samples. In view of the results a possible mechanism of this
ionic-polarization is discussed.

20.

THEORETICAL STUDIES ON THE EXCITATION OF THE VISIBLE DAYGLOW
by
Edward C. Zipf, Jr., Assistant Professor of Physics

*   *   *

ROCKET MEASUREMENTS OF THE VISIBLE DAYGLOW*

ABSTRACT

        Recent rocket measurements of the spectrum and altitude
distribution of the visible dayglow are reviewed. The current theory
of the dayglow is discussed in the light of these data and the
results of new laboratory studies on atomic processes of aeronomic
interest. The important role played by solar radiation in the
excitation of the visible dayglow is illustrated in a detailed
discussion of the emission of the (0,0) negative band of N_2^+ and the
red line (6300 A) of atomic oxygen in the dayglow.

* In press, Journal of Geomagnetism and Geoelectricity.

21.

COMMUNICATION BY ELECTRICAL STIMULATION OF THE SKIN
by
Robert H. Gibson, Associate Professor of Psychology

General

This is a program of psychophysical experiments with electrical pulse stimulation of the skin senses. The rationale is described in the previous report of this series. Progress has involved primarily the following projects: numbered as in the previous report:

Projects

1. Multiple Dimension Stimulus Control System

A system was designed around a photo-block paper tape reader to control and deliver combinations of multiple electric stimuli to several locations on the body surface. Two of the six channels now have operated in full for the first time. The further, and hopefully the final problems to be solved prior to use include getting the logic to reset reliably after each stimulus.

3. Skin Temperature Effects on Touch and Pain Sensitivity

The basic problem has been to determine effects of temperature on electrically aroused cutaneous sensations. Skin surface temperature has been varied (see previous report) by means of an electrical thermode attached to machined brass electrodes. Effects of temperature again were found to be slight on electrically aroused touch, this time with long trains of pulses.

Finding only slight effects on touch with electric stimuli might result either from the fact that effects indeed are slight or nonexistent thereby implying direct stimulation of the nerves themselves, or from the thermal diffusitivity of and the absorption pattern within the skin being such that the temperature changes at the electrode-skin interface are not mirrored over time within the receptor tissue layers.

As a first step in clarifying the nature of radiant energy transfer through human tissues, the lateral temperature gradient was measured along the surface of the web between thumb and index finger. For five minutes, a 15 mm. diameter electrode was maintained at 18° C., 15° C below normal surface temperature at an ambient temperature of 70° F. The surface gradient obtained with a 5 mm. diameter thermistor is steep, the temperature only several millimeters from the edge of the electrode being within 2.8° C. of the normal temperature. Therefore, although it is likely that the heat rise within the tissues grows over time as the linear square root of the surface temperature, we need to determine the thermal inertial constants for inner

tissues. Either subsurface temperature measurements should be done, or some other procedure used based partly on lateral surface gradients. The crucial question is the real depth at which little further temperature change occurs for large step changes in surface temperature.

4. Electrical Properties of Tissue

As stinging pain from electrical stimulation of hairy tissues might reflect tissue breakdown, systematic increases in peak current were monitored separately and photographed from four separate oscilloscope traces for four parallel segments of an electrode fed by a single constant current stimulator. The point was to determine whether aspects of current flow through a given segment relative to the other three were related to pain appearance. The data have not yet been sufficiently analyzed to comment.

6. Equal "Loudness" Functions

The study introduced in the previous report is in its final stages. Threshold and equal "loudness" functions are being obtained from three observers as a function of (i) train duration, (ii) pulse repetition rate, (iii) electrode size, and (iv) body region. Data collection will be completed early in May.

Appendix A

NASA Predoctoral Trainees

	Name	BS/BA from	Department	Quality Point Average* (A = 4.00)
1.	William Abkemeier	St. Louis	Elect. Eng.	3.58
2.	Marshall Abrams	Carnegie Tech	Elect. Eng.	3.16
3.	Ronald Coffield	Pittsburgh	Mech. Eng.	3.61
4.	William Coffman	Thiel	Biology	3.85
5.	James Cope	West Virginia	Mech. Eng.	3.57
6.	George Delancey	Pittsburgh	Chem. Eng.	3.86
7.	Paul Demmie	Pittsburgh	Physics	3.20
8.	George Doschek	Pittsburgh	Physics	4.00
9.	David Emin	Florida State	Physics	3.46
10.	John Farrell**	Baldwin-Wallace	Chemistry	3.71
11.	Bruce Fike	Union	Elect. Eng.	3.69
12.	Leo Geary	Pittsburgh	Elect. Eng.	3.42
13.	William Greger	Lafayette	Elect. Eng.	3.58
14.	Richard Hake, Jr.	Cal Tech	Physics	3.20
15.	Philip H. Harju	N. Dakota	Chemistry	3.37
16.	Nancy Heatwole	Madison	Chemistry	3.70
17.	Donald Jessep, Jr.	Pittsburgh	Elect. Eng.	4.00
18.	William Johnson	Brigham Young	EPS***	3.81
19.	Patrick Kokoska	Pittsburgh	Chem. Eng.	3.49
20.	Paul A. Kossey	Pittsburgh	Elect. Eng.	3.66
21.	John Lyons	Loyola (Chicago)	Psychology	3.41
22.	James McKearney	Long Island	Psychology	4.00
23.	George Mosteller	Pittsburgh	Elect. Eng.	3.58
24.	Joseph Natowitz**	Florida	Chemistry	3.58
25.	Edward J. Nemeth	Pittsburgh	Chem. Eng.	3.31
26.	Robert L. Nielsen	Penn State	Physics	3.27
27.	David Opferman	Penn State	Elect. Eng.	3.40
28.	Rafael Perez	New Mexico State	Elect. Eng.	3.76
29.	Joel Peterson	Penn State	Mech. Eng.	3.55
30.	Edward Phillips	Lafayette	Chem. Eng.	3.15
31.	James Pommersheim	Pittsburgh	Chem. Eng.	3.78
32.	Charles Richter	St. Joseph's	Physics	3.40
33.	Charles R. Seeger	Ohio State	EPS***	3.54
34.	Anthony Sobota	Indiana (Pa.)	Biology	3.90
35.	Charles Springer	Swarthmore	Chemistry	3.71
36.	Nunzio Tartaglia	Manhattan	EPS***	3.91
37.	Brian K. Thomas	Reed	Physics	3.20
38.	William Tilton	Pittsburgh	Mech. Eng.	3.19
39.	Raymond Turner	Carnegie Tech	Physics	3.28
40.	David Uhrich	Canisius	Physics	3.57
41.	Felix Ullrich	Rutgers	Physics	3.33
42.	Charles S. Weller	M.I.T.	Physics	3.18
43.	John Zelik	Pittsburgh	Physics	3.43
			Average	3.54

* For trainees enrolling in September 1965 this is the undergraduate QPA; for all others it is the graduate QPA.

** Completed the requirements for the Ph.D.

*** Earth and Planetary Sciences

APPENDIX B

NASA Postdoctoral Research Associates

(name in parentheses is that of the cognizant faculty member)

Name	Year	Ph.D. From	Program
Helmut Ankel (Prof. D. S. Feingold)	1960	Univ. Marburg, Germany	Polysaccharide synthesis of _Cryptococcus laurentii_
R. K. Duggins (Prof. C. C. Yates)	1962	Univ. Nottingham, England	Theoretical study of flow separation
Felix Franks (Prof. H. S. Frank)	1958	Univ. London	Interpretation of properties of aqueous solutions in terms of the two-fluid model of liquid water
Elli O. Hand (Prof. T. Cohen)	1962	Harvard Univ.	Study of reactions in heterocyclic compounds in which radicals serve as intermediates
Watson R. Henderson (Prof. W. Fite)	1963	Univ. Texas	Electron collisions with excited atoms and molecules
Edgar Inselberg (Prof. J. Rosenberg)	1962	Univ. Illinois	Photosynthesis studies; re-examination of statistical analysis of radio-assay
Truman H. Jordan (Prof. G. A. Jeffrey)	1964	Harvard Univ.	The investigation of the crystal structure of $H_2CO_3.Ef_2O$; the construction of an automated single crystal diffractometer
Kotu Lulla (Prof. T. Donahue)	1964	New York Univ.	Laboratory study of upper atmosphere atomic interactions, particularly charge exchange processes

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APPENDIX B - continued

Name	Ph.D. From	Year	Program
Thomas Mak (Prof. G. A. Jeffrey)	Univ. British Columbia	1963	Mode of formation of crystalline hydrates from gases; applications to planetary atmosphere studies
Jack L. Pinkus (Prof. T. Cohen)	Univ. Southern Calif.	1956	Study of solvolytic reactions in ammonia in which carbonium ions are intermediates
M. Schlesinger (Prof. J. Anderson)	Hebrew Univ., Jerusalem	1963	Optical absorption and thermoluminescence in materials containing color centers
John Tanaka (Prof. J. Carter)	Iowa State Univ.	1956	Chemical and structural studies of inorganic-aromatic complexes; electron-deficient bonding in aluminum alkyls
S. Venketeswaran (Prof. C. Partanen)	Univ. Pittsburgh	1961	Study of radiation effects on albino mutants of tobacco cells to understand the mechanism of photosynthesis
William Vogt	Univ. Pittsburgh	1962	Studies of solid-state electronic devices